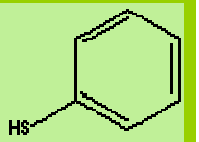
THIOPHENOL



PRODUCT IDENTIFICATION	
CAS NO.	108-98-5
EINECS NO.	203-635-3
FORMULA	C_6H_5SH
MOL WT.	110.17
H.S. CODE	2930.90
TOXICITY	Oral, rat LD50: 46200 ug/kg
SYNONYMS	Phenylmercaptan; Benzenethiol; Mercaptobenzene;
DERIVATION	
CLASSIFICATION	

PHYSICAL AND CHEMICAL PROPERTIES	
PHYSICAL STATE	Colorless or pale yellow liquid
MELTING POINT	-15 C
BOILING POINT	168 - 169 C
SPECIFIC GRAVITY	1.073
SOLUBILITY IN WATER	Insoluble (soluble in alcohol and ether)
pH	
VAPOR DENSITY	3.80
AUTOIGNITION	
REFRACTIVE INDEX	1.5880
NFPA RATINGS	
FLASH POINT	50 C
STABILITY	Stable under normal conditions. Oxidizes when exposed to air

APPLICATIONS

Mercaptan: any of a class of organosulfur compounds is similar to the alcohol and phenol but containing a sulfur atom in place of the oxygen atom. Compounds containing -SH as the principal group directly attached to carbon are named 'thiols'. In substitutive nomenclature their names are formed by adding '-thiol' as a suffix to the name of the parent compound. When -SH is not the principal group, the prefix 'mercapto-' is placed before the name of the parent compound to denote an unsubstituted -SH group. 'thio' is a chemical prefix indicates the replacement of an oxygen in an acid radical by sulfur with a negative valence of 2. Sulfur analog of alcohol is called thiol (or mercaptan), and ether analog is called sulfide.

The first chemical contrast of thiols and sulfides with alcohols and ethers is acidity which is important in organic reactions. Thiols are stronger acids than relevant alcohols and phenols. Thiolate conjugate bases are easily formed, and are excellent nucleophiles in SN2 reactions of alkyl halides and tosylates. The nucleophilicity of sulfur is much greater than that of oxygen, resulting in a number of useful electrophilic substitution reaction that are rare by oxygen. For example, sulfides form (with alkyl halides) ternary sulfonium salts, in the same alkylattion of tert-amines quaternary ammonium salts, whereas ternary oxonium salts are prepared only under extream conditions. Without exception, sulfoxides, sulfinate salts and sulfite anion also alkylate on sulfur, despite of the partial negative formal charge on oxygen and partial positive charge on sulfur. The second character is the oxidation states of sulfur. Oxygen has only two oxidation states, whereas sulfur covers from –2 to +6 as follows:

- -2: Hydrogen Sulfide (H_2S), sulfides, sulfonium ions

- -1: disulfides
- 0: S elemental, sulfoxides, sulfenic acids
- +2: sulfones, sulfinic acids
- +4: sulfonic acids, sulfite esters
- +6: sulfate esters

One more sulfur compound's contrast with oxygen analog is in oxidation chemistry. Oxidation of sulfur compounds changes the oxidation state of sulfur rather than carbon, whereas, oxidation of alcohols to aldehydes and ketones changes the oxidation state of carbon not oxygen. Thiol is oxidized to S-S single bond (disufide) which is stronger than O–O bond in peroxide. Disufide forms sulfenyl chlorides (with chlorine in mild condition) or sulfonic acids under harder condition. Oxidation of sulfides with hydrogen peroxide (or peracids) yields sulfoxides and then to sulfones. A certain sulfoxide compound such as dimethyl sulfoxide can be used as an effective oxygen source in the oxidation reaction of primary and secondary alcohols to aldehydes and ketones. DMSO easily is reduced to dimethyl sulfide and water is taken up by the electrophile. oxidation procedure is very mild and tolerates a variety of other functional groups, including those having oxidizable nitrogen and sulfur atoms.

Thiophenol is a compound of aromatic thiol which is structurally analogous to phenol; hydroxyl group (-OH) bonded to the aromatic ring is replaced by a sulfhydryl group (-SH). This structure means that the oxygen atom hydroxyl group is replaced by a sulfur atom. Thiophenol is also calledphenyl mercaptan. Thiophenol is a toxic, flammable clear liquid with a strong and disagreeable odor; boiling at 168 C. It is insoluble in water but soluble in alcohol and ether. Many chemical reactions of thiophenols are analogous to phenols. The substantial difference between sulfur and oxygen is that sulfur much more readily gets oxidized to higher oxidation states than oxygen. Sulfur in organic compounds is fairly stable in several oxidation states. Thiophenols can form thiophenolate anions by losing sulfhydryl H+ ions; used as reagents for the simple chemical preparation. The ring closure reaction of *o*-amino thiophenol produces benzothiazole, animportant industrial product. Thiophenol itself is used as an antinematodal agent. Thiophenol class compounds have the skeleton of thiophenol.

SALES SPECIFICATION	
APPEARANCE	Colorless or pale yellow liquid
ASSAY	98.0% min
TRANSPORTATION	
PACKING	200kgs in Drum
HAZARD CLASS	6.1
UN NO.	2337
OTHER INFORMATION	